1H-Indene, 2-methyl-2177-47-1 | DTXSID00176173

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75	Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.87	0.81	0.87	0.82	0.86	0.86	

Model Results

Predicted value: 2.44e-04 mol/L

Global applicability domain: Inside

Local applicability domain index: 6.12e-01

Confidence level: 6.00e-01

Nearest Neighbors from the Training Set

Image not found

5-Ethylidene-2-norbornene

Measured: 7.40e-05 Predicted: 2.32e-04

Image not found

Hexachlorocyclopentadiene

Measured: 6.60e-06 Predicted: 9.10e-06

Image not found

Diethyl disulphide Measured: 2.45e-03 Predicted: 3.63e-03

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4-Pentenyl isothiocyanate

Measured: 1.26e-03 Predicted: 1.49e-03